Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 302 °C

Global applicability domain: Outside

Local applicability domain index: 2.73e-01

Confidence level: 5.04e-01

Nearest Neighbors from the Training Set

Image not found
Ethyl oxanilate
Measured: 280
Predicted: 295

Image not found
Phenacetin
Measured: 244
Predicted: 301

Image not found
Propanil
Measured: 351
Predicted: 317

Image not found
N-(4-Methoxyphenyl)acetamide
Measured: 335
Predicted: 303

Image not found
N-(2-Methoxyphenyl)acetamide
Measured: 304
Predicted: 301